Journal of the Arab American University مجلة الجامعة العربية الامريكية للبحوث

Volume 2 | Issue 2 Article 3

2016

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Abstract

In this paper, a periodic One-Component Plasma (OCP) system of N-point particles is simulated by Monte Carlo (MC) technique in three dimensions. Because of the long range nature of the Coulomb potential, no cut-off distance is considered in calculations (i.e, for each particle i, the effect of the other N-1 particles on i, is taken into account). The maximum allowed displacement "dmax" used in MC simulation controls the convergence to the equilibrium state of the system. An optimum maximum allowed displacement, O-dmax, is found and is given by a function of the temperature and the density of the system. Obtaining this function is done statistically by fitting the calculated data resulted from simulating the system at different values of temperature and density. The obtained O-dmax gives fast convergence of the simulation.

Keywords: *One component plasma, optimum, allowed displacement, Monte Carlo.*

Introduction

The OCP is a system of *N*-identical charged particles interacting through Coulomb potential and embedded in a uniform compensating background of opposite charge. The OCP in one, two, and three dimensions explores the features and properties of many phenomena in the fields of electrodynamics, statistical mechanics, and thermo-dynamics. Hence, it has been under focus by many researchers in the last six decades (Levesque D. W. J., 1983), (Deutsch C., 1974), (B. J. , 1981), (Alstuey A, Surface properties of the three-dimensional one-component plasma, 1981), (L., 2004), (Zambrodin A., 2006). The bulk and surface properties of the three dimensional OCP were studied using MC simulation (Levesque D. W. J., 1983). The structure of strongly coupled uniform OCP in two and three dimensions is calculated by the "Onsager Molecule" approach (Rosenfield Y., 1989). Simple analytical approximations for the internal energy of the strongly coupled OCP in two and three dimensions are studied in (Kharpak Sergy A., 2014). The fermion MC variational calculations were performed to determine the equation of state of the uniform OCP in two and three dimensions (D, 1972). The magnetic properties of the OCP in two and three dimensions were studied in (Alstuey A, Magnetic properties of a nearly classical one component plasma in three or two dimensions, 1980).The general variational formulation for the application of Mean Spherical Approximation for soft potentials, and the results of the OCP were discussed and extended in (Y., 1984). The equilibrium properties of the classical OCP in a uniform background of opposite charge were computed for systems of various sizes using MC method (J., 1973). At one special temperature, the equilibrium statistical mechanics of the classical two dimensional OCP were worked out exactly in (B. J. , 1984). MC computations of the surface energy of the classical OCP have been made for different values of the plasma parameter Gamma (Badiali J. P., 1983). The MC simulation was used to study the lattice dynamics in the harmonic approximation and the solution of the hyper-netted-chain equation in the classical two dimensional OCP (Gann R. C.Chakravarty, 1979). Results from MC study of the classical two dimensional OCP were obtained in (Brush1 V. M., 1966), (Caillo1 J. M., 1982). The fluctuations in the net electric charge in a two dimensional OCP with uniform background charge density were studied using computational simulations (Levesque D. W. J., 2014). The two dimensional OCP Yukawa systems in a perpendicular magnetic field was studied using computational technique to explore the equilibrium particle dynamics in the fluid state (Ott T.,

2014). Many other references can be found in the literature that study different systems of OCP. In this research, the OCP in three dimensions is studied using Metropolis MC, (MMC) method. The aim of the research is to obtain an explicit formula that gives the O-d_{max} as a function of temperature and density. The same methodology has been used for Lennard Jones (Al-Shraydeh, 2015). Obtaining such a displacement and using it in simulation will decrease the computational work needed to reach the equilibrium state of the system. In the next section, we will present the MMC simulation method. The effect of the choice of d_{max} on calculations will be discussed in section 3. Numerical results will be presented in section 4, and a fitting of the data will be done in order to obtain the O-d_{max} for any choice of temperature and density. Discussion, conclusions, and future perspectives will be made in the last section.

Monte Carlo Simulation

Monte Carlo (MC) is considered to be the most important simulation techniques that are usually used for solving problems in statistical physics. In MC method, the basic idea is to evaluate thermal averages of materials by statistically sampling a desired region of the phase space of a model using computers (Newman M. E. J., 1999). The quick development of computational resources, and the expansion of new algorithms allow MC simulations to be a base for studying lots of subjects of statistical physics (M., 1992). The results obtained in this work are based on MC simulations. Hence, a brief look at the general idea behind equilibrium thermal MC techniques is done in this section. In any *N*-particle system with constant volume V, constant temperature T, and constant number of particles *N* (NVT ensemble), the average value <*A*> of any observable *A* of the system can be approximated by (Landua D. P., 2000).

$$\bar{A} = \frac{1}{M}\sum_{i=1}^{M} A(t_i), \tag{1}$$

Where *M* is the number of the sampled points from the distribution P(t), and t_i denotes the configuration *i* of the system. The distribution P(t) is

$$P(t) = \frac{e^{-\beta U(t)}}{\int e^{-\beta U(t)} dt}, \tag{2}$$

where β = 1/(KBT), KB is the Boltzmann constant and U is the potential total. Practically, it is possible to construct a Markov chain of configurations $t_{1,}$ $t_{2...}$ t_n that approaches the desired distribution P (t). This construction can be done using a technique developed by Metropolis and co-workers in 1953 and the Metropolis Monte Carlo (MMC) (Metropolis N., 2008). This technique depends on the fact that the probability of transferring the system from state t_i to state t_j is (David M. Ferguson, 1999), (AR, 2004)

$$Pr(ti \rightarrow tj) = \min\{1, e^{-\beta\Delta U}\}, \quad (3)$$

Where $\Delta U = U(t_j)\text{-}U(t_i)$.

Metropolis *et.al.*, suggested the following steps in order to determine whether the change of the state of the periodic *N*-particle system will be accepted or rejected.

1. Choosing randomly the initial state, t_i, of the system.
2. Enumerating the particles from *1* to *N*. Let *k =1*.
3. While *k <N*, doing steps 5-12.
4. Calculating the total potential energy U_i.
5. Generating a new state, t_j, by changing the position of particle k.
6. Calculating the new total potential energy U_j.
7. Computing the difference in the energy $\Delta U = U_j\text{-}U_i$.
9. Calculating the transition probability P_r according to equation (3).
10. Generating a uniform distribution random number, ξ , in the interval [0; 1].
11. If Pr ($t_i \rightarrow t_j$) is greater than ξ , accept the move, let j = i and k = k + 1, otherwise, reject the move and let k = k + 1. Go to step 5.
12. Repeating steps (3- 12) N_s times, where N_s denotes the number of MC sweeps.

Increasing the number of MC sweeps, N_s will increase the accuracy of calculating the desired properties of the system. Each move of any particle at each MC sweep must obey the periodicity of the system; the reason is that the physical system under consideration is infinite. Number of particles in the center box is *N* (Figure 1). All other boxes are copies of the central one. When a particle moves outside this box, an alternative particle enters it from the opposite side. Moving the particles, the researcher must do the simulation according to a criterion that does not allow the particle's displacement to exceed a limited value. This criterion is discussed in the next section.

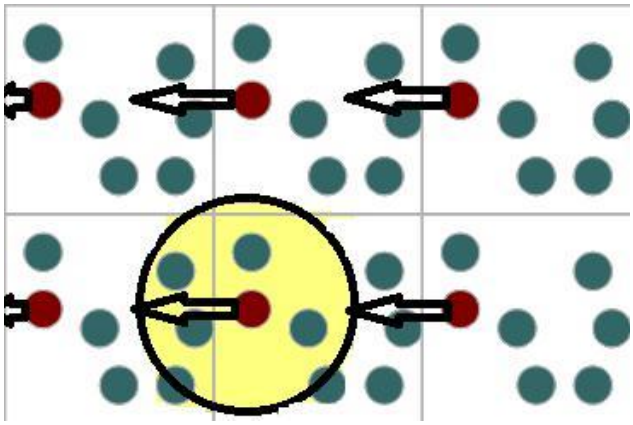

Figure 1: The periodicity of the N-particle system.

Maximum Allowed Displacement

The random movements in step 5 of the MMC algorithm determines the acceleration of convergence to the equilibrium state of the system. The random displacement of any particle is given by

$$\vec{\delta} = d_{max} . (\vec{1} - 2.\vec{\xi}) \quad (4)$$

where d_{max} is the maximum allowed displacement of the particle along the coordinate axes, $\vec{1}$=(1, 1, 1), and $\vec{\xi}$ is a vector whose components are random numbers distributeduniformly on the interval [0, 1]. The acceptance rate (the ratio between the numbers of the accepted moves to all number of moves ($N*N_s$)) depends on d_{max}. If $\vec{r}_i^{old}$ is the position of the particle before movement, then, the new position, taking into account the periodicity, is given by

$$\vec{r}_i^{new} = \vec{r}_i^{old} + \vec{\delta} \quad (5)$$

If the particle's movements are too small, neighboring configurations will be highly correlated and any essential change of the configuration will need many particle displacements. If d_{max} is too large, most moves will be rejected, which will also lead to the increase of the computational work. In our research we will determine the best d_{max} at any given temperature and density. The criteria that will be used are the speed of convergence to the equilibrium state. In many systems other than OCP, it was found that the d_{max} corresponds to acceptance rate of *50%*, which is common, although there is no motivation that this value is optimal.

Numerical Results

A periodic OCP system of fixed N particles, fixed temperature T, and fixed volume V is simulated in three dimensions using MMC technique (NVT-MC). The number of particles used in calculations is 125 particles, which is traditionally sufficient to get the desired results. The number of MC sweeps used is N_s=10000 which is statistically enough. Because of the long range nature of the system, a large dimensionless scale cube box of five length edge is used, and no cut-off distance is considered in calculations.

The potential function of the OCP system is the Coulomb one, which is given by

$$f(r_{ij}) = \frac{1}{4\pi\epsilon_o}\frac{q_i q_j}{r_{ij}} \tag{6}$$

Where r_{ij} is the distance between the two particles i and j, (in our system, $q_i = q_j$ for all$i$ and j), the constant $\in_o$ is the electrical permittivity of space. The reduced form of the Coulomb potential which is considered in our calculations is

$$f(r^*_{ij}) = \frac{1}{r^*_{ij}}, \tag{7}$$

Where

$$r^*_{ij} = \frac{4\pi\epsilon_o}{q_i q_j} r, \tag{8}$$

The temperature T is also given in reduced form

$$T^* = TK_B, \tag{9}$$

While the density is

$$\rho^* = \frac{N}{V}, \tag{10}$$

The NVT-MC code was written in C^{++} language using C^{++} builder 6 and tested on Windows 2007, 32 bit. Once the simulation runs stable measurements of respective energy is performed. The output data files were saved in Microsoft Excel format and the output figures were saved as output Matlab figures. The reason for installing C^{++} builder 6 instead of the other builders is that, it could be linked directly with Matlab 2008, and Microsoft Office Excels 2010. In NVT-MC code, the right balance between readability, taking advantage of C^{++} features, and performance have been considered in this work. The Coulomb potential energy behavior of the point particles,

which simulated in 3D lattice, is studied to obtain the O-d_{max} that leads to get fast equilibration optimally with minimum number of MC sweeps. During the simulation, the calculations of the Coulomb potential followed the expected physical behavior, and the periodic boundary conditions worked correctly. The simulation was done using different values of temperature T and density in the ranges [0.5, 3], and [0.25, 2] respectively. The convergence of the Coulomb potential as a function of MC sweeps is tested. The values of d_{max} associated with faster convergence, O-d_{max}, are listed in tables 1, 2, 3, 4, 5, and 6.

Table 1: The values of O-d_{max} at T^*=1.0

ρ^*	O-d_{max}
0.2500	0.039117567
0.3125	0.032716157
0.3750	0.028504404
0.4375	0.025380106
0.5000	0.023230942
0.6250	0.020190683
0.7500	0.017987165
1.0000	0.015327276
1.2500	0.013626067
1.5000	0.012557762
1.7500	0.010328764
2.0000	0.009598112

Table 2: The values of O-d_{max} at T^* =1.0

ρ^*	O-d_{max}
0.2500	0.211217788
0.3125	0. 173166707
0.3750	0. 146356671
0.4375	0. 128675012
0.5000	0. 114926428
0.6250	0. 096981353
0.7500	0. 085340521
1.0000	0. 069153823
1.2500	0. 057870671
1.5000	0. 048931762
1.7500	0. 042939171
2.0000	0. 038454244

Table 3: The values of O-d_{max} at T^* =1.5

ρ^*	O-d_{max}
0.2500	0. 928200925
0.3125	0. 724771376
0.3750	0. 587099005
0.4375	0. 496245599
0.5000	0. 415476390
0.6250	0. 313707649
0.7500	0. 252662978
1.0000	0. 209657745
1.2500	0. 164118476
1.5000	0. 136255572
1.7500	0. 116671792
2.0000	0. 102599723

Table 4: The values of O-d_{max} at T^* =2.0

ρ^*	O-d_{max}
0.2500	2.453771943
0.3125	1.897912977
0.3750	1.551728904
0.4375	1.290991592
0.5000	1.237715042
0.6250	0.878966628
0.7500	0.712006513
1.0000	0.515461608
1.2500	0.387777545
1.5000	0.317012074
1.7500	0.256496178
2.0000	0.219619119

Table 5: The values of O-d_{max} at T^* =2.5

ρ^*	O-d_{max}
0.2500	1.934964176
0.3125	1.797793148
0.3750	1.686102781
0.4375	1.632385194
0.5000	1.574118315
0.6250	1.506529980
0.7500	1.461528562
1.0000	1.282053425
1.2500	1. 200022068
1.5000	1.121495183
1.7500	1.077586427
2.0000	0.500460792

Table 6: The values of O-d_{max} at T^* =3.0

ρ^*	O-d_{max}
0.2500	2.327120570
0.3125	2.150301425
0.3750	2.021993410
0.4375	1.899782981
0.5000	1.823846144
0.6250	1.728136450
0.7500	1.607847958
1.0000	1.486817400
1.2500	1.424641803
1.5000	1.333967768
1.7500	1.079311682
2.0000	0.924562430

Figure 2 shows an example of the Coulomb potential versus MC sweeps at different values of d_{max} at specific temperature and density and the acceptance rate associated with the O-d_{max} which is about 50%. This fact is true for all values of T**;** Figure 3 shows the fitted curve of the O-d_{max} as a function of density for specific temperature; it decreases by increasing the density; figure 4 shows that the behavior of O-d_{max} as a function of density at different values of temperature**;** Figure 5 shows the best fitting curve of the O-d_{max} as a function of temperature at specific density**;** Figure 6 shows the simulating results of O-d_{max} as a function of temperature at different values of density. Clearly, the O-d_{max} increases by increasing the temperature of large densities. For small densities, results show the same conclusion for temperature less than two; Figure 7 is a 3-dimensional fitted curve that gives the O-d_{max} as a function of temperature and density. The data is taken from Tables 1, 2, 3, 4, 5, and 6. Fitting the data is done by Matlab and gives the following explicit mathematical formula**:**

$$F(T^*,\rho^*) = 0.5733 - 0.6203*T^* - 1.57*\rho^* + 1.226*T^{*2} - 1.211*T^**\rho^* + 2.051*\rho^{*2} - 0.2482\,T^{*3} + 0.2031*T^{*2}*\rho^* + 0.08202*T^**\rho^{*2} - 0.5642*\rho^{*3}, \quad (11)$$

where F(T^*, ρ^*) represents the O-d_{max} at any T and . The correlation coefficient for Formula 11 is 0.95.

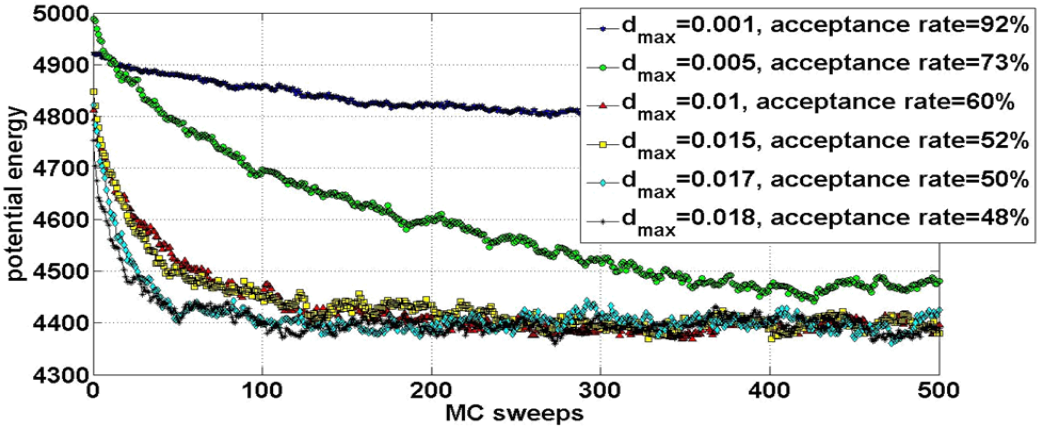

Figure 2: The Coulomb potential versus MC sweeps at T^* =0.5.

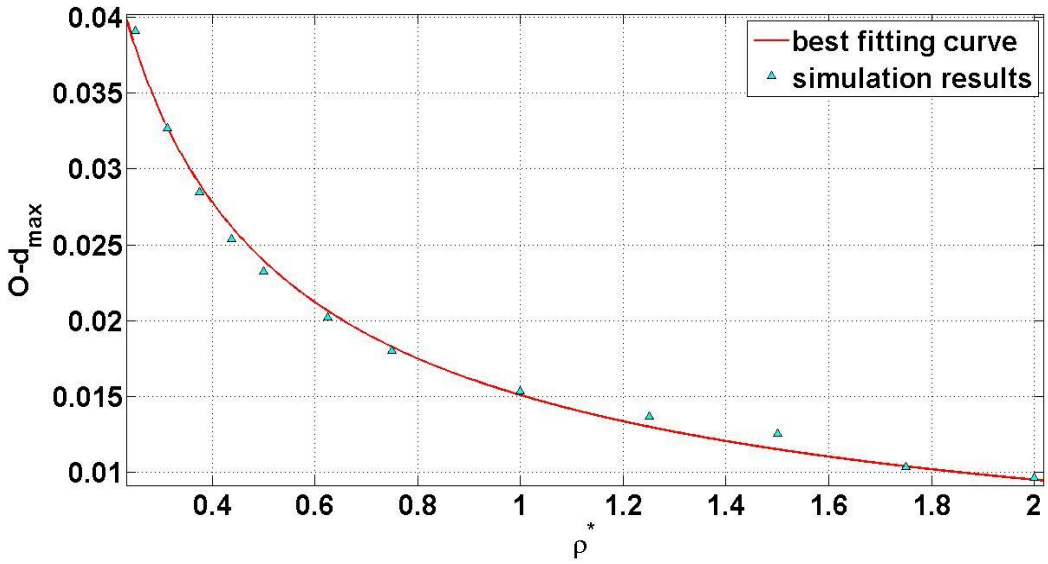

Figure 3: The O-d_{max} versus ρ^* at $T^* = 0.5$

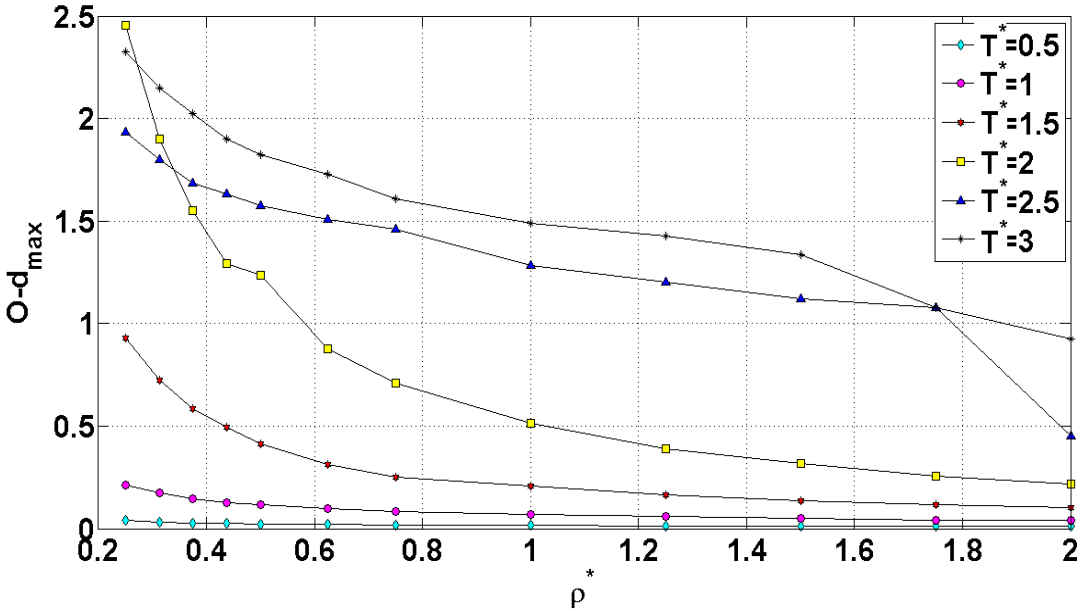

Figure 4: The O-d_{max} versus ρ^* at different values of T^*.

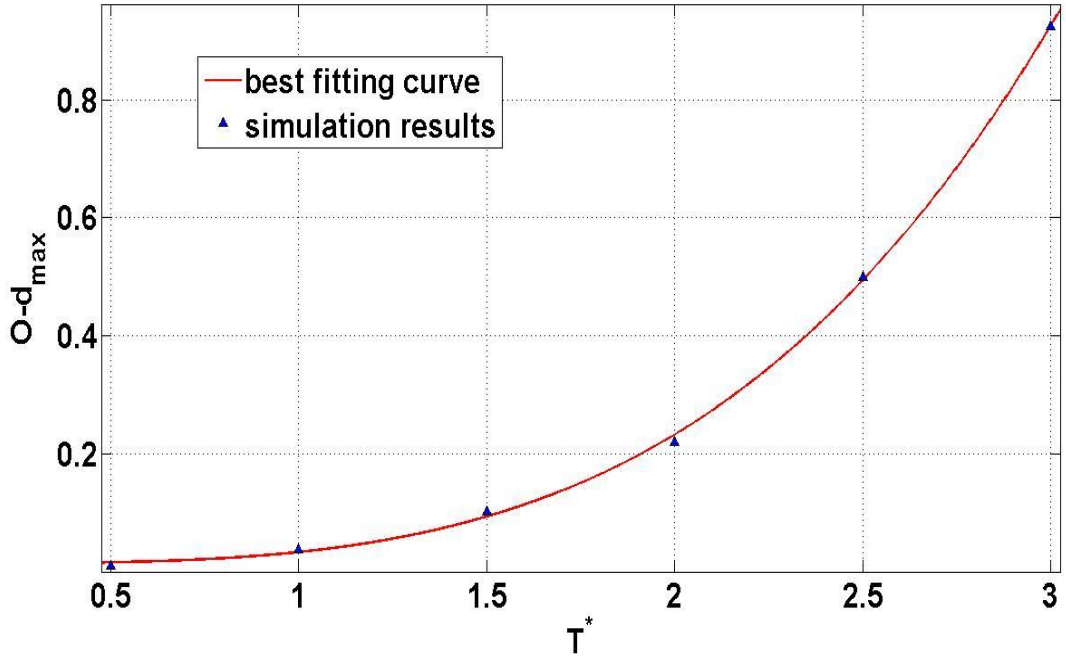

Figure 5: The O-d_{max} versus T^* at $\rho^* = 2$.

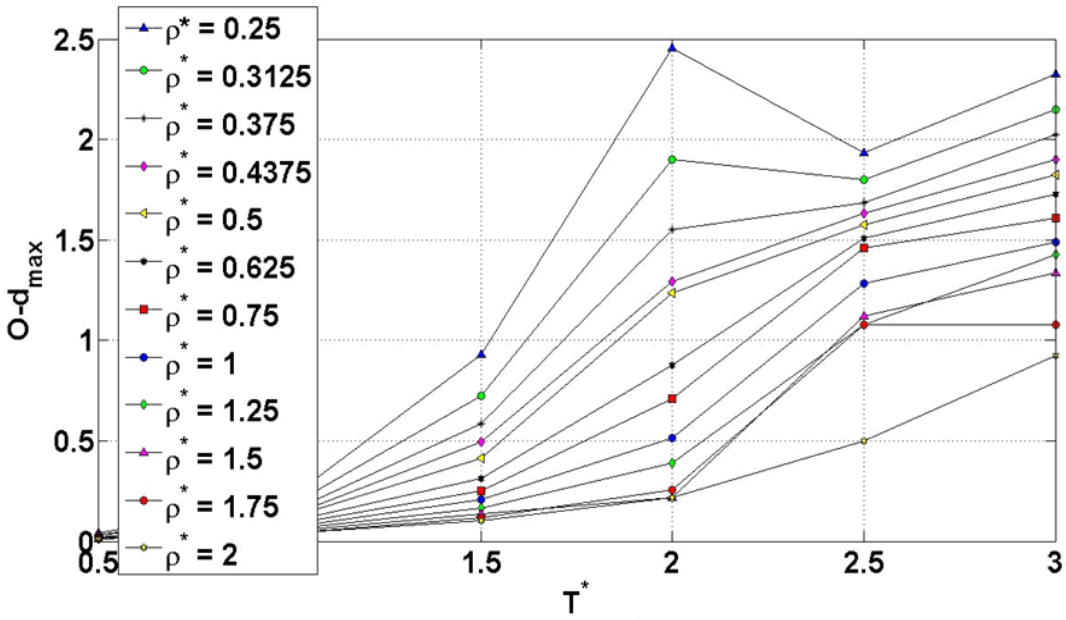

Figure 6: The O-d_{max} versus T^* at different values of ρ^*.

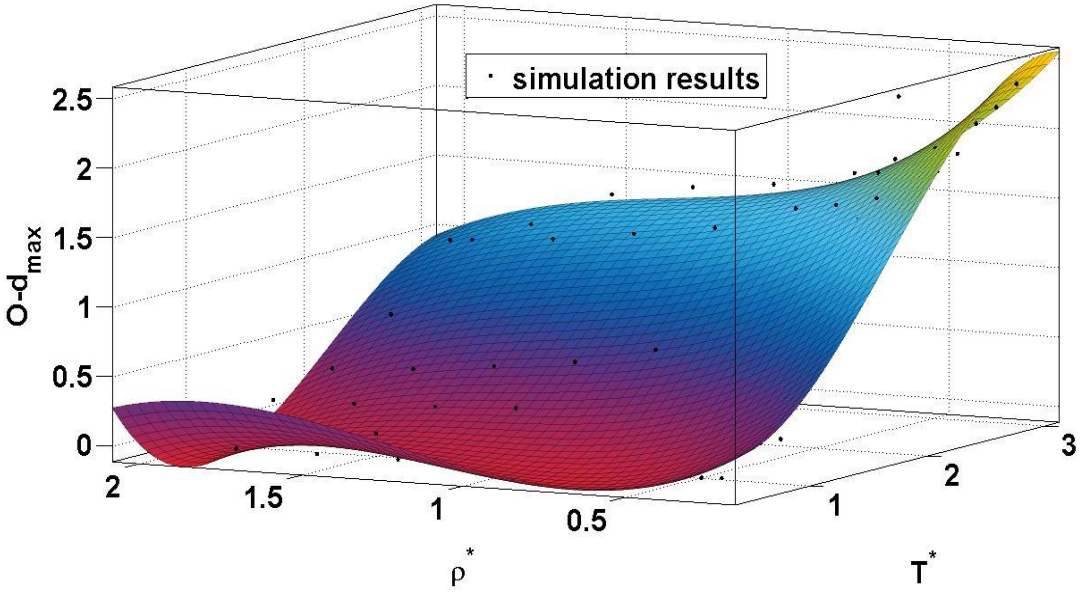

Figure 7: The best fitted surface that represents the O-d_{max} as a function of temperature and density.

Conclusions and Future Work

The OCP is considered as one of the most important systems that occur in many phenomena in science. The metropolis MC simulation method has been used very often in the last six decades in order to understand the properties of those systems. The speed of convergence of the simulation to the equilibrium state of the system is affected by many parameters like number of particles, density, temperature, and maximum allowed displacement d_{max}. In this research, an optimum d_{max} is obtained as a function of temperature and density for fixed number of particles. The formula obtained is given by 11 with correlation coefficient 0.95. In any OCP systems, an MC simulation can be done efficiently by using the O-d_{max} obtained in this research. As a future work, we are planning to add kinetic energy calculations and take in our consideration the radius of atom to apply the simulation at real systems. Moreover, we will incorporate the dipole-dipole interactions in the OCP system, and the optimum maximum allowed displacement of the angle and check out the relation between the best angle and the best displacement. The two Component Plasma will also be under focus in a future work.

References

1. Al-Shraydeh, H. H. (2015). Lennard-Jones Molecules Using the Monte Carlo Simulations with Optimum Maximum Allowed Displacement, MSc thesis. Palestine: Arab American University.
2. Alstuey A, J. B. (1980). Magnetic Properties of a Nearly Classical One Component Plasma in Three or Two Dimensions. Elsevier B V, Volume 102, issue 2, 327-343.
3. Alstuey A, J. B. (1981). Surface Properties of the Three-Dimensional One-Component Plasma. J Phys (France), 42, 1.
4. AR, A. (2004). Monte Carlo Simulation for Classical Two-Dimensional Dipolar Antiferromagnetic Systems on a Square Lattice. Canada: St. John's Newfoundland and Labrador.
5. B., J. (1981). Surface Properties of the Three-Dimensional One-Component Plasma. Phys. Rev. Lett., 46, 386.

6. B., J. (1984). Statistical Mechanics of Defense Ionized Matter. I. Equilibrium Properties of the Classical One-Component Plasma. Journal of Statistical Physics, 34(5-6), 803-815.
7. Badiali J. P., R. M. (1983). Surface Density Profile of the One-Component Plasma. Journal of Physics C: Solid State Physics Volume 16.
8. Brush1 V. M., S. H. (1966). Monte Carlo Study of One-Component Plasma. I. J. Chem. Phys. 45, 2102.
9. Caillo1 J. M., L. D. (1982). A Monte Carlo Study of the Classical Two-Dimensional One-Component Plasma. Journal of Statistical Physics , 28(2), 325-349.
10. D, C. (1972). Ground State of the Fermion One-Component Plasma: A Monte Carlo Stusy in Two and Three Dimensions. Phys. Rev. B, 18, 3126.
11. David M. Ferguson, I. J. (1999). Monte Carlo Methods in Chemical Physics. John Wiley and Sons, 105, 245.
12. Deutsch C., L. M. (1974). Surface Properties of the Three-Dimensional One-Component Plasma. Phys. Rev. A, 9, 2598.
13. Gann R. C.Chakravarty, S. G. (1979). Monte Carlo Simulation of the Classical Two-Dimensional One-Component Plasma. Phys. Rev. B, 20, 326.
14. J., H. (1973). Statistical Mechanics of Defense Ionized Matter. I. Equilibrium Properties of the Classical One-Component Plasma. Phys. Rev. A, 8, 3096.
15. Kharpak Sergy A., K. A. (2014). Simple Thermodynamics of Strongly Coupled One-Component-Plasma in Two and Three Dimensions. Phys. Plasma, 21, 104-505.
16. L., S. (2004). Surface Properties of the Three-Dimensional One-Component Plasma. J. Stat. Phys., 117, 131.
17. Landua D. P., B. K. (2000). A Guide to Monte Carlo Simulations in Statistical Physics. Cambridge University Press.
18. Levesque D., W. J. (1983). Surface Properties of the Three-Dimensional One-Component Plasma. Journal of Statistical Physics, 33(3), 549-557.
19. Levesque D., W. J. (2014). Charge Fluctuations in the Two-Dimensional One-Component Plasma. Journal of Statistical Physics, 100(1-2), 209-222.
20. M., B. V. (1992). Long-Range Order in a Classical Two-Dimensional Dipole System. Journal of Physics: Condensed Matter, 4, 75-82.

21. Metropolis N., R. A. (2008). Fundamentals of Statistical and Thermal Physics. J. Chem. Phys., 21, 1087.
22. Newman M. E. J., B. G. (1999). Monte Carlo Methods in Statistical Physics. Clarendon Press.
23. Ott T., L. H. (2014). Dynamic of Two-Dimensional One-Component Plasma and Binary Yukawa in a Magnetic Field. Phys. Rev. E., 89.
24. Rosenfield Y., L. D. (1989). "Onsager-Molecule" Approach to Liquid Structure: The One-Component Plasma in Two and Three Dimensions. Phys. Rev. A., 39, 3079.
25. Y., R. (1984). Comments on the Mean Spherical Approximation for Hard-Core and Soft Potentials and an Application to the One-Component Plasma. Journal of Statistical Physics, 37(1-2), 215-236.
26. Zambrodin A., W. P. (2006). Surface Properties of the Three-Dimentional One-Component Plasma. J. Phys. A., 39, 8933.

أفضل ازاحة قصوى ممكنة في محاكاة مونتي كارلو لنظام البلازما ذات المكون الوحيد

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الملخص

ينهض هذا البحث بمحاكاة نظام مكرر متعدد من جزيئات البلازما ذات المكون الوحيد في الفضاء ثلاثي الأبعاد، وذلك باستخدام تقنية مونتي كارلو؛ بسبب طبيعة جهد كولوم بعيد التأثير، وفي هذا البحث لم يتم اعتبار جهد القطع في الحسابات (تم الأخذ بعين الاعتبار تأثير كل جزيء على الآخر)، تتحكم الازاحة القصوى الممكنة للجزيء والمستخدمة في محاكاة النظام باستخدام مونتي كارلو بسرعة التقاء جزيئات النظام الى منطقة الجهد المتعادل، إن افضل ازاحة قصوى ممكنة حسبت وتم ايجاد اقتران رياضي مرتبط بدرجة الحرارة والكثافة للنظام. ثم الحصول على الأقتران الرياضي بملاءمة البيانات المحسوبة من محاكاة النظام عند درجات حرارة وكثافة مختلفة؛ لايجاد أفضل إزاحة قصوى التي تعطي تقارب سريع للمحاكاة.

الكلمات الدالة: *جزيئات البلازما ذات المكون الوحيد، أفضل إزاحة قصوى، محاكاة مونتي كارلو.*